07/08/200316:25Print selected from Online session

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FILE COVERS 1907 - 7 Aug 2003 VOL 139 ISS 6 FILE LAST UPDATED: 6 Aug 2003 (20030806/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> macrocyclic

18359 MACROCYCLIC

84 MACROCYCLICS

L11 18390 MACROCYCLIC

(MACROCYCLIC OR MACROCYCLICS)

=> serine()protease()inhibitor

90472 SERINE

1452 SERINES

91032 SERINE

(SERINE OR SERINES)

76425 PROTEASE

28810 PROTEASES

89502 PROTEASE

(PROTEASE OR PROTEASES)

418585 INHIBITOR

441774 INHIBITORS

679145 INHIBITOR

(INHIBITOR OR INHIBITORS)

L12 2794 SERINE (W) PROTEASE (W) INHIBITOR

=> hepatitis()C()virus

39020 HEPATITIS .

3061941 C

285727 VIRUS

61717 VIRUSES

296084 VIRUS

(VIRUS OR VIRUSES)

L13 8183 HEPATITIS (W) C (W) VIRUS

=> 11 and 12 and 13

18359 MACROCYCLIC

84 MACROCYCLICS

18390 MACROCYCLIC

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(MACROCYCLIC OR MACROCYCLICS)
             0 COUMPONDS
             0 MACROCYCLIC (W) COUMPONDS
         18359 MACROCYCLIC
            84 MACROCYCLICS
         18390 MACROCYCLIC
                 (MACROCYCLIC OR MACROCYCLICS)
       753760 COMPOUNDS
       1500776 COMPDS
       1895912 COMPOUNDS
                 (COMPOUNDS OR COMPDS)
          5256 MACROCYCLIC(W) COMPOUNDS
        718326 13
L14
            0 L1 AND L2 AND 13
=> 12 and 13
         18359 MACROCYCLIC
            84 MACROCYCLICS
         18390 MACROCYCLIC
                 (MACROCYCLIC OR MACROCYCLICS)
        753760 COMPOUNDS
       1500776 COMPDS
       1895912 COMPOUNDS
                 (COMPOUNDS OR COMPDS)
          5256 MACROCYCLIC (W) COMPOUNDS
             2 HEPETITIS
       3061941 C
             1 HEPETITIS (W) C
             0 L2 AND L3
L15
=> 111 and 112 and 113
             2 L11 AND L12 AND L13
L16
=> d all 1-2
L16 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
     2001:798207 CAPLUS
AN
     135:344735
     Preparation of macrocyclic NS3-serine protease
     inhibitors of hepatitis C virus
     comprising alkyl and aryl alanine p2 moieties
     Venkatraman, Srikanth; Chen, Kevin X.; Arasappan, Ashok; Njoroge, F.
IN
     George; Girijavallabhan, Viyyoor M.; Chan, Tin-Yau; McKittrick, Brian A.;
     Prongay, Andrew J.; Madison, Vincent S.
PA
     Schering Corporation, USA
SO
     PCT Int. Appl., 218 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
     ICM C07D273-00
IC
     34-3 (Amino Acids, Peptides, and Proteins)
     Section cross-reference(s): 1, 7, 63
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                      KIND DATE
     PATENT NO.
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                            _____
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A3
PΙ
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                            20020801
     WO 2001081325
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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             TJ, TM
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                            20000419
     WO 2001-US12530
                       W
                            20010417
OS
     MARPAT 135:344735
GΙ
```

Macrocyclic compds. I [E, X, Y may be independently present or
absent, and if present may be (un)substituted (cyclo)alkyl, aryl,
heteroalkyl, heteroaryl, ether, amino, sulfide, sulfone, amide,
sulfonamide, urea, carbamate, hydrazide, carbonyl, etc.; R1 = acyl or
boryl groups; Z = O, N, or CH; W = null, CO, CS, SO2, C:NR (R = H, alkyl,
cycloalkyl, aryl, etc.); Q = (NR)p (p = 0-6), O, S, CH2, CHR, CRR' (R' =
any group given for R) or a double bond toward V; A = O, CH2, (CHR)p,
(CHRCHR')p, (CRR')p, NR, S, SO2, CO or a bond; G = (CH2)p, (CHR)p,

II

```
(CRR')p, NR, O, S, SO2, SO2NH, CO or a bond towards E or V; R2, R3, R4 =
     H, (un) substituted (hetero) alkyl, -aryl or -cycloalkyl, alkoxy, aryloxy,
     alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate,
     urea, ketone, aldehyde, cyano, nitro, etc.], including enantiomers and
     pharmaceutically acceptable salts, were prepd. as hepatitis
     C virus (HCV) protease inhibitors. Thus, peptide II was
     prepd. by a multistep procedure involving cyclization of intermediate
     cyclopentadiene-.eta.6-ruthenium-4-chlorophenylpropionic
     acid-cyclohexylglycine-m-tyrosine-OMe. II showed Ki = 0.001-1.0.mu.M in
     the HCV protease assay. The invention also discloses pharmaceutical
     compns. comprising I as well as methods of using them to treat disorders
     assocd. with the HCV protease.
ST
     macrocyclic peptide prepn NS3 serine protease
     inhibitor; hepatitis C treatment macrocyclic peptide
ΙT
     Hepatitis
        (C; prepn. of macrocyclic NS3-serine
        protease inhibitors of hepatitis C
        virus)
IT
    .Peptides, preparation
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (cyclic; prepn. of macrocyclic NS3-serine
        protease inhibitors of hepatitis C
        virus)
IΤ
     371110-87-1P
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     371111-19-2P
                    371111-23-8P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (prepn. of macrocyclic NS3-serine protease
        inhibitors of hepatitis C virus)
ΙT
     371110-88-2P
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                                  371110-92-8P
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    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of macrocyclic NS3-serine protease
        inhibitors of hepatitis C virus)
ΙT
    149885-80-3
    RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (prepn. of macrocyclic NS3-serine protease
        inhibitors of hepatitis C virus)
    298-12-4, Glyoxylic acid 627-00-9, 4-Chlorobutyric acid
                                                                 627-05-4,
    1-Nitrobutane 821-41-0, 5-Hexen-1-ol
                                             867-13-0, Triethyl
    phosphonoacetate
                       1119-60-4, 6-Heptenoic acid
                                                    1745-17-1
                                                                 2019-34-3
    3601-66-9 6282-88-8, Benzenepropanol, 4-chloro-
                                                        7389-87-9
    30515-28-7, 7-Bromoheptanoic acid 34087-14-4 68090-88-0
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ΙT

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123053-23-6
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    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
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        (prepn. of macrocyclic NS3-serine protease
       inhibitors of hepatitis C virus)
IT · 371112-06-0P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of macrocyclic NS3-serine protease
       inhibitors of hepatitis C virus)
L16 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
    2001:763001 CAPLUS
AN
DN
    135:318715
    Preparation of macrocyclic NS3-serine protease
     inhibitors of hepatitis C virus
     comprising n-cyclic p2 moieties
    Chen, Kevin X.; Arasappan, Ashok; Venkatraman, Srikanth; Parekh, Tejal N.;
ΤN
    Gu, Haining; Njoroge, F. George; Girijavallabhan, Viyyoor M.; Ganguly,
    Ashit; Saksena, Anil; Jao, Edwin; Yao, Nanhua H.; Prongay, Andrew J.;
    Madison, Vincent S.; Vibulbhan, Bancha
PΑ
    Schering Corporation, USA
SO
    PCT Int. Appl., 402 pp.
    CODEN: PIXXD2
DT
    Patent
LΑ
    English
IC
    ICM C07D498-00
     34-3 (Amino Acids, Peptides, and Proteins)
     Section cross-reference(s): 1, 63
FAN.CNT 1
                 KIND DATE
                                        APPLICATION NO. DATE
     PATENT NO.
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OS
      MARPAT 135:318715
GI
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- Title compds. I [wherein X and Y = independently (cyclo)alkyl, heteroalkyl, (aryl)heteroaryl, alkyl(hetero)aryl, substituted ether, sulfide, sulfone, amide, sulfonamide, urea, carbamate, hydrazide, carbonyl, etc.; R1 = CHO, acyl, or (un) substituted carboxy, carbamoyl, boryl, etc.; Z = O, N, or CH, W = null or CO, CS, or SO2; Q = null or CH, N, P, (CH2)p, (CHR)p, (CRR')p, O, NR, S, or SO2; A = O, CH2, (CHR)p, (CHRCHR')p, (CRR')p, NR, S, SO2, or a bond; E = CH, N, CR, or a double bond toward A, L, or G; G = null or (CH2)p, (CHR)p, or (CRR')p; J = nullor CH, CR, O, S, or NR; M = null or O, NR, S, SO2, "(CH2)p, (CHR)p, (CHRCHR')p, or (CRR')p; p = 0-6; R, R', R2, R3, and R4 = independently H, (cyclo)alkyl, alkenyl, heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate, urea, ketone, CHO, CN, NO2, O, N, S, P, etc.] were prepd. as hepatitis C virus (HCV) protease inhibitors. For example, II (multi-step prepn. given) was cyclized, deesterified, and coupled with III.bul.HCl (prepn. given) to give the macrocyclic hydroxyamide intermediate. Oxidn. using Des-Martin reagent followed by flash chromatog. afforded two diastereomers IV in 82% combined yield. The (S)-isomer inhibited NS3-serine protease HeLa/Huh7 co-transfected cells with a Ki of 2 .mu.M. The invention also discloses pharmaceutical compns. comprising I as well as methods of using them to treat disorders assocd. with the HCV protease.
- ST macrocyclic peptide prepn NS3 serine protease inhibitor; peptide macrocycle prepn hepatitis C treatment IT Hepatitis
 - (C, treatment; prepn. of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)
- Peptides, preparation
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

IT study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)

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study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (prepn. of macrocyclic NS3-serine protease
   inhibitors of hepatitis C virus
   comprising cyclic p2 moieties)
149885-80-3, NS3 serine protease
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
(Biological study); PROC (Process)
   (prepn. of macrocyclic NS3-serine protease
   inhibitors of hepatitis C virus
   comprising cyclic p2 moieties)
367259-40-3P
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367259-45-8P
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367259-50-5P
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RL: PEP (Physical, engineering or chemical process); SPN (Synthetic
preparation); PREP (Preparation); PROC (Process)
   (prepn. of macrocyclic NS3-serine protease
   inhibitors of hepatitis C virus
   comprising cyclic p2 moieties)
98-58-8, 4-Bromobenzenesulfonyl chloride
                                           98-61-3, Pipsyl chloride
99-06-9, 3-Hydroxybenzoic acid, reactions
                                           107-87-9, 2-Pentanone
108-46-3, 1,3-Benzenediol, reactions 621-37-4
                                                  627-05-4, 1-Nitrobutane
1013-88-3, Diphenylketimine
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                                                               1119-60-4,
6-Heptenoic acid
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                               2900-27-8
                                           2905-24-0, 3-
Bromobenzenesulfonyl chloride
                               4248-19-5, tert-Butyl carbamate
4724-10-1
            4799-68-2, 3-Benzyloxypropanol
                                             13726-69-7
                                                          19721-22-3,
3-Mercaptopropanol
                    19790-60-4, 3-Benzyloxypropionaldehyde
                                                              27516-53-6,
Pentenoic acid
                32462-30-9
                                           36805-97-7
                              33821-94-2
                                                        39687-95-1, Methyl
                               64187-48-0
isocyanoacetate
                  58558-53-5
                                            74844-93-2
                                                         77530-32-6
             102195-79-9
                                         109183-71-3
                           103262-83-5
78183-55-8
                                                       109183-72-4
             131721-90-9
121148-00-3
                            161879-12-5
                                          367260-42-2
                                                        367260-44-4
367260-47-7
              367260-49-9
                            367260-51-3
                                          367260-53-5
                                                        367260-55-7
367260-57-9
              367260-62-6
                            367260-64-8
                                          367260-67-1
                                                        367260-69-3
367260-71-7
              367260-73-9
                            367260-76-2
                                          367260-78-4
                                                        367260-80-8
                                          367260-94-4
367260-82-0
              367260-87-5
                            367260-90-0
                                                        367260-96-6
367260-99-9
              367261-01-6
                            367261-07-2
                                          367261-09-4
                                                        367261-12-9
                            367261-22-1
367261-14-1
              367261-20-9
                                          367261-24-3
                                                        367261-26-5
367261-28-7
              367261-30-1
                            367261-32-3
                                          367261-35-6
                                                        367261-38-9
367261-40-3
              367261-44-7
                            367261-46-9
                                          367261-48-1
                                                        367261-50-5
                            367261-54-9
367261-51-6
              367261-52-7
                                          367261-56-1
                                                        367261-58-3
367261-66-3
              367261-69-6
                            367261-71-0
                                          367261-73-2
                                                        367261-75-4
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368454-24-4
                   368454-26-6
                                  368871-37-8
                                                368871-38-9
                                                               368871-39-0
     368871-40-3
                   368871-41-4
                                  368871-42-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of macrocyclic NS3-serine protease
        inhibitors of hepatitis C virus
        comprising cyclic p2 moieties)
     69651-48-5P
IT
                   74844-91-0P
                                  84520-67-2P
                                                84740-98-7P
                                                               88931-77-5P
     119927-71-8P
                    166196-05-0P
                                    166196-06-1P
                                                   204398-85-6P
                                                                   367258-42-2P
     367258-43-3P
                    367258-44-4P
                                    367258-45-5P
                                                   367258-46-6P
                                                                   367258-47-7P
     367258-48-8P
                    367258-49-9P
                                    367258-50-2P
                                                   367258-51-3P
                                                                   367258-52-4P
     367258-53-5P
                    367258-54-6P
                                    367258-55-7P
                                                   367258-56-8P
                                                                   367258-57-9P
     367258-58-0P
                    367258-59-1P
                                    367258-60-4P
                                                   367258-61-5P
                                                                   367258-62-6P
     367258-63-7P
                    367258-64-8P
                                    367258-65-9P
                                                   367258-66-0P
                                                                   367258-67-1P
     367258-69-3P
                    367258-70-6P
                                    367258-72-8P
                                                   367258-73-9P
                                                                   367258-75-1P
     367258-77-3P
                    367258-79-5P
                                    367258-82-0P
                                                   367258-83-1P
                                                                   367258-85-3P
     367258-86-4P
                    367258-87-5P
                                    367258-88-6P
                                                   367258-89-7P
                                                                   367258-92-2P
     367258-95-5P
                    367258-97-7P
                                    367258-98-8P
                                                    367258-99-9P
                                                                   367259-01-6P
     367259-02-7P
                    367259-03-8P
                                    367259-04-9P
                                                   367259-05-0P
                                                                   367259-06-1P
     367259-07-2P
                    367259-08-3P
                                    367259-09-4P
                                                    367259-10-7P
                                                                   367259-11-8P
     367259-12-9P
                    367259-13-0P
                                    367259-14-1P
                                                   367259-15-2P
                                                                   367259-16-3P
     367259-17-4P
                    367259-18-5P
                                    367259-19-6P
                                                    367259-20-9P
                                                                   367259-21-0P
     367259-22-1P
                    367259-23-2P
                                    367259-24-3P
                                                    367259-25-4P
                                                                   367259-26-5P
     367259-27-6P
                    367259-28-7P
                                    367259-29-8P
                                                    367259-30-1P
                                                                   367259-31-2P
     367259-32-3P
                    367259-33-4P
                                    367259-34-5P
                                                   367259-35-6P
                                                                   367259-36-7P
     367259-37-8P
                    367259-38-9P
                                    367259-39-0P
                                                   367259-59-4P
                                                                   368454-16-4P
     368454-18-6P
                    368454-20-0P
                                    368454-22-2P
                                                   368871-11-8P
                                                                   368871-12-9P
     368871-13-0P
                    368871-14-1P
                                    368871-15-2P
                                                    368871-16-3P
                                                                   368871-17-4P
     368871-18-5P
                    368871-19-6P
                                    368871-20-9P
                                                    368871-21-0P
                                                                   368871-23-2P
     368871-24-3P
                    368871-25-4P
                                    368871-26-5P
                                                    368871-27-6P
                                                                   368871-28-7P
     368871-29-8P
                    368871-30-1P
                                    368871-31-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of macrocyclic NS3-serine protease
        inhibitors of hepatitis C virus
        comprising cyclic p2 moieties)
     87691-27-8P
ΙT
                   121147-97-5P
                                   121148-05-8P
                                                  149507-31-3P
                                                                  367259-52-7P
                                    367259-57-2P
     367259-54-9P
                    367259-56-1P
                                                   367259-58-3P
                                                                   367259-60-7P
     367259-61-8P
                    367259-62-9P
                                    367259-63-0P
                                                   367259-64-1P
                                                                   367259-65-2P
     367259-66-3P
                    367259-67-4P
                                    367259-68-5P
                                                   367259-70-9P
                                                                   367259-72-1P
     367259-74-3P
                    367259-76-5P
                                    367259-79-8P
                                                   367259-81-2P
                                                                   367259-85-6P
     367259-87-8P
                    367259-89-0P
                                    367259-91-4P
                                                   367259-93-6P
                                                                   367259-95-8P
     367259-97-0P
                    367259-99-2P
                                    367260-01-3P
                                                   367260-04-6P
                                                                   367260-06-8P
                    367260-10-4P
     367260-08-0P
                                    367260-12-6P
                                                   367260-14-8P
                                                                   367260-15-9P
     367260-17-1P
                    367260-19-3P
                                    367260-22-8P
                                                   367260-24-0P
                                                                   367260-27-3P
     367260-29-5P
                    367260-31-9P
                                    367260-33-1P
                                                   367260-35-3P
                                                                   367260-36-4P
     367260-38-6P
                    367261-83-4P
                                    367264-98-0P
                                                   368871-32-3P
                                                                   368871-33-4P
     368871-34-5P
                    368871-35-6P
                                    368871-36-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of macrocyclic NS3-serine protease
        inhibitors of hepatitis C virus
        comprising cyclic p2 moieties)
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